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Fall 2021

CHE 342-001: Chemical Engineering Thermodynamics II

Gennady Gor

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1. **ChE 342 - Chemical Engineering Thermodynamics II**

2. **Credits and contact hours:** 3-0-3 (3 lecture hr/wk - 0 lab hr/wk - 3 course credits)

3. **Course Coordinator or Instructor:** Gennady Gor

4. **Textbook:** Fundamentals of Chemical Engineering Thermodynamics, Kevin D. Dahm, Donald P. Visco, Cengage Learning, (2014). ISBN: 1111580707

5. **Specific course information**

a. **Description:** The principles and methods developed in Chemical Engineering Thermodynamics I are extended to multicomponent systems, and used to treat phase and chemical equilibrium as well as such applications as chemical reactors and refrigeration systems.

b. **Prerequisites:** ChE 230, Math 211 (or Math 213), Chem 236

c. **Required, Elective, or Selective Elective** - Required

6. **Specific goals for the course**

a. A student should be able to:

1. Calculate efficiencies for reversible and practical cycles, such as Carnot, Rankine & Brayton
2. Calculate heat absorption and heat rejection rates for cycles
3. Calculate work of turbines & pumps
4. Analyze internal combustion engines & gas turbine engines
5. Analyze refrigeration cycles & liquefaction processes
6. Apply Raoult's law and Henry's law to solve thermodynamics problems
7. Predict behavior from liquid/vapor phase diagrams including azeotropes
8. Carry out bubble and dew point calculations for a given mixture
9. Calculate partial properties of binary solutions, such as partial molar volumes
10. Calculate activity coefficients using correlating equations such as Margules and Lan Laar
11. Determine VLE using ideal gas and ideal solution models
12. Analyze appropriate models for calculating phase equilibrium
13. Interpret phase diagrams of binary systems
14. Calculate vapor-liquid equilibria for non-electrolyte systems
15. Predict equilibrium compositions of mixtures under phase equilibria
16. Apply concepts of equilibria of multi-component, multi-phase systems to the evaluation and design of separation processes, such as distillation
17. Estimate the fugacity coefficients for given mixtures
18. Analyze ideal gas/solution models that reflect behavior of real mixtures based on concepts of excess free energy and chemical potential

b. This course explicitly addresses the following student outcomes: 1

7. **Topics**

1. Heat Engines
2. Refrigeration Processes
3. Vapor-Liquid Equilibrium
4. Solution Thermodynamics
5. Solution Thermodynamics Applications
6. Chemical Reaction Equilibria

ChE 342: Chemical Engineering Thermodynamics II

Fall 2021

Instructor: Dr. Gennady Gor, Assistant Professor

Office/Lab: 357/321A Tiernan Hall, Phone: 973-596-2944, E-mail: gor@njit.edu

Teaching Assistant: Ruosong Dong, Ph.D. student, E-mail: rd466@njit.edu;

Gbenga Ladapo, Ph.D. student, E-mail: ggl3@njit.edu

Class: Tuesday, Thursday, 1:00-2:20 PM; Room: GITC 1100

Office Hours: Tuesday, Thursday 2:30-3:30 AM; Room: 373 Tiernan Hall

Additional appointments can be made by email.

Course Web Page: <https://njit.instructure.com/courses/18831>

Course Description and Requirements

This course will cover heat engines, refrigeration, thermodynamics of mixtures, phase equilibrium and chemical-reaction equilibrium. Solid knowledge of chemical engineering thermodynamics including these topics is necessary to succeed in more advanced chemical engineering courses. In particular, the current course is a pre-requisite for ChE 349 Kinetics and Reactor Design and ChE 360 Separation Processes I.

Pre-Requisites: ChE 230, Math 211 (or Math 213), Chem 236

Course Objectives

Taking this course, a motivated student will learn to:

- Use the laws of thermodynamics to analyze basic power and refrigeration cycles.
- Apply both fundamental and practical knowledge of thermodynamics to the design of basic power and cooling cycles.
- Apply concepts of thermodynamics to solutions.
- Determine equilibrium compositions of chemical reaction products and two-phase liquid/vapor mixtures.

Learning Materials

Textbook Required: Fundamentals of Chemical Engineering Thermodynamics, Kevin D. Dahm, Donald P. Visco (2014). ISBN: 1111580707

Additional: Introduction to Chemical Engineering Thermodynamics, Seventh Edition, J.M. Smith, H.C. Van Ness and M.M. Abbott, McGraw-Hill (2005). ISBN: 0-07-310445-0

Other Learning Material: The textbook is the main source for preparing for classes and reading the textbook before each class is necessary. Additional materials will be posted on Canvas

<https://njit.instructure.com/courses/18831>

Students are strongly encouraged to use LearnChemE.com website for preparing to concept quizzes:

<http://www.learncheme.com/screencasts/thermodynamics>

Calculator: A high-end calculator (TI-83, TI-84 or TI-84SE) is required for solving homework, quiz, and exam problems.

Computer: Students have to bring their laptops to every class. The laptops' batteries have to be charged, as power outlets will not necessarily be available. In-class activities and quizzes will

require use of laptop computers. In-class use of computers at times other than for in-class activities or quizzes is not permitted.

Software: Excel of similar software is necessary to work on some of the computational assignments. Use of Matlab, Python or other computational software is strongly recommended for working on homework assignments.

Course Outline

Class	Date	Topic (preliminary, subject to changes)
1	Sep. 2	Recollection of Thermo I and PChem
2	Sep. 7	Carnot Cycle (PV and TS diagram).
3	Sep. 9	Rankine Cycle.
4	Sep. 14	Vapor Compression Refrigeration Cycle.
5	Sep. 16	PH -diagrams. Examples.
6	Sep. 21	Examples on Refrigeration.
7	Sep. 23	Basics of Liquefaction. Joule-Thomson Process.
8	Sep. 28	Liquefaction. Linde and Claude Processes.
9	Sep. 30	Phase Equilibrium for Pure Components: Gibbs Free Energy.
10	Oct. 5	Midterm 1.
11	Oct. 7	Phase Equilibrium for Pure Components: Vapor Pressure.
12	Oct. 12	Chemical Potential and Fugacity.
13	Oct. 14	Fugacity from EOS. Poynting Method.
14	Oct. 19	Introduction to Mixtures.
15	Oct. 21	Properties of Mixing. Partial Molar Properties.
16	Oct. 26	Partial Molar Properties of Binary Mixtures.
17	Oct. 28	Pxy and Txy Diagrams. Raoult's law. Bubble and Dew Points Calculations.
18	Nov. 2	Dew T calculation. Two-component PT Flash. Lever Rule.
19	Nov. 4	Midterm 2.
20	Nov. 9	Three-component Flash. Modified Raoult's Law. VLE Calculation Based on it.
21	Nov. 11	Phase Equilibrium for Mixtures. Mixture Fugacity.
22	Nov. 16	Raoult's and Henry's Laws from Mixture Fugacities.
23	Nov. 18	Fugacity from Generalized Correlations and Virial EOS.
24	Nov. 23	Gibbs Free Energy Models. One- and Two-parameter Margules Equation.
	Nov. 25	<i>Thanksgiving. No Class.</i>
25	Nov. 30	Data Reduction Procedure Using Margules Equation.
26	Dec. 2	Wilson and Van Laar Equations. Thermodynamic Consistency. Integral Test.
27	Dec. 7	Basics of Chemical Reactions Equilibrium.
28	Dec. 9	P and T Effects on Reaction Equilibrium. Van't Hoff Equation.

Assessment and Grading

Homework: Homework assignments will be given regularly, at least ten assignments per semester. The assignments will be posted on Canvas. The homework (including both reading and problems assignments) must be completed within a week, unless otherwise is explicitly stated. E.g. if the homework is assigned on Tuesday it is due before the next Tuesday's class. Most homework will

not be collected, and will be assessed through the in-class quizzes. The reading assignments will be assessed through the concept quizzes. However, some of the homework assignment can be collected randomly and graded. In this case, no late homework will be accepted.

Quizzes: Regular quizzes will be given based on the homework material, including both concepts and problems. The quizzes will not be announced in advance, so please be prepared to have a quiz during every class. No make-up quizzes will be allowed. All quizzes will be closed book with no material allowed. The quizzes will often take place at the beginning of the class, so being on time is strongly encouraged. Online quizzes will be proctored using the Respondus and other tools used by NJIT, see <https://ist.njit.edu/respondus>.

Exams: There will be two midterm exams and one final exam. The final exam will be cumulative. All exams will be closed book, however a handwritten formula sheet (double-sided, letter size) for midterm exams will be allowed. The formula sheet may only include formulas and notes about their application. You may not include worked-out problems on your formula sheet. Formula sheets will be collected with the exam. For the final exam two sheets are allowed.

Homeworks & Quizzes	25%
Midterm #1	20%
Midterm #2	25%
Final Exam	30%
	100%

Percent	Grades
$\geq 85\%$	A
$\geq 80\%$	B+
$\geq 75\%$	B
$\geq 70\%$	C+
$\geq 65\%$	C
$\geq 55\%$	D
$< 55\%$	F

Important Dates

- Midterm exam #1: October 5, 2021
- Midterm exam #2: November 4, 2021
- Final exam: between December 15 and 21, 2021
- Withdraw Deadline: November 10, 2021

Policies

Statement on Academic Integrity: (as formulated by Provost Deek) “Academic Integrity is the cornerstone of higher education and is central to the ideals of this course and the university. Cheating is strictly prohibited and devalues the degree that you are working on. As a member of the NJIT community, it is your responsibility to protect your educational investment by knowing and following the academic code of integrity policy that is found at: <http://www5.njit.edu/policies/sites/policies/files/academic-integrity-code.pdf>.

Please note that it is my professional obligation and responsibility to report any academic misconduct to the Dean of Students Office. Any student found in violation of the code by cheating,

plagiarizing or using any online software inappropriately will result in disciplinary action. This may include a failing grade of F, and/or suspension or dismissal from the university. If you have any questions about the code of Academic Integrity, please contact the Dean of Students Office at dos@njit.edu”

Special Needs: If you need accommodations due to a disability please contact Chantonette Lyles, Associate Director of Disability Support Services, Fenster Hall Room 260 to discuss your specific needs. A Letter of Accommodation Eligibility from the Disability Support Services office authorizing your accommodations will be required.

Lectures

- Attendance is strongly recommended. The examples discussed in the class are not necessarily from the main textbook and therefore missing a class will have consequences for preparation to quizzes and exams. Attendance will be taken through record on participation in in-class activities.
- The classes start at 1:00, and the students must be in class by that time. Being late to class may have consequences for the grade, since many of the classes will start from quizzes.
- Electronic devices other than calculators (laptops, tablets, cell-phones etc.) are not permitted during the classes. No audio or video recording is allowed.
- Laptops will be permitted only if necessary for in-class activities.
- No audio or video recording is allowed.
- Cellphones should be turned off during both lectures and exams and not allowed unless specifically permitted by the instructor.
- No eating any time during the classes.

Course materials, office hours and correspondence

- The course Canvas page is the main platform for delivering information about the course. All relevant course materials and assignments will be posted on Canvas, so a student should check it regularly: <https://njit.instructure.com/courses/18831>
- The students have to upload a professional-looking head shot for their Canvas profile.
- The students are strongly encouraged to use the Canvas discussion boards corresponding to each of the modules.
- The students are strongly encouraged to attend Office Hours held bi-weekly. Long questions, which require derivations will be discussed only during the Office Hours and will not be answered by email. Questions regarding grades can be discussed only during the Office Hours.
- E-mail is the preferred way for correspondence with the instructor.
- E-mail and Canvas correspondence is intended only for quick questions. Questions which require a detailed discussion should be discussed during the Office Hours.
- All correspondence should be conducted in a professional style, using formal English.
- To assure quick response to your emails, please add “ChE342” in the subject of your emails.
- The instructor reserves the right not to respond to emails if the email does not have a greeting or a signature.

Exams, Quizzes, Homeworks and Grades

- A letter grade is based on the final score, calculated using an Excel spreadsheet in accordance with the Tables given in this syllabus. The assigned letter grade is final and cannot be negotiated.

- There is no curve.
- A student can dispute the exam scores within a week after the announcement of the score. Exam scores can be disputed during the official Office Hours, not during class time or via email.
- Students will get zero for not coming to quizzes, exams, or any other course activity. If students miss an exam due to extreme circumstances (such as a medical problem), they need to notify the instructor via email before the beginning of the exam, and bring proof of the circumstance to the Dean of Student's office. Only in the case of official approval from the Dean of Student's office, may a make-up be given at the discretion of the instructor.
- A student must show as many details when solving a problem during an exam or a quiz. Not showing the work will cause losing points even if the final answer is correct.
- Partial credits can be given for solving the exams problems.
- No partial credit will be given if there is not enough details to follow.
- The final answer should be always evaluated with respect to its reasonability. No partial credit will be given if the final answer is wrong and unreasonable, and it is not stated.
- There will be no partial credits for the questions/problems on quizzes.
- The grade for quizzes will be calculated based on $N - 2$ best quizzes, where N is the number of all quizzes within the semester. Typically $10 \leq N \leq 12$. Therefore, one can miss up to two quizzes and, if the remaining quizzes are still get the whole 25% for the quizzes part of the grade.
- If a student misses a quiz due to a legitimate reason (absence approved by the Dean of Students), this quiz is excluded from the calculation, and the weights of the quizzes are scaled proportionally.
- Student handwriting must be legible in order to receive points.
- A student coming to dispute a grade has to bring completed homework sheets. No discussion of grades will be held without completed homework.

Format for Completing Assignments

- Writing Mechanics - All completed assignments should be carefully and legibly printed. If it cannot be read, it cannot be graded.
- Calculations - All calculations should be consistent with the following.
 - Include complete calculations for every calculation presented to demonstrate how results were obtained.
 - Include all units for each term in each equation. The units must balance.
 - Use the appropriate number of significant figures: typically three, but not exceeding the number of significant figures in the given data.
 - Clearly indicate the final solution by boxing it in with a rectangle.
- Problem Order - Problems should be clearly labeled, and presented in the order assigned (one, two, three, etc.).
- Problem Essentials - Problem solutions should include the following items in order.
 - Problem number listed at the beginning of the problem.
 - Brief problem statement. Provide bullet points of key aspects of the problem if it is longer than a few sentences.
 - The required information - the information or solution that we are looking for.
 - A straight-edge or carefully drawn diagram(s) that clearly illustrates the problem. Optional, but often needed.

- The boxed solution of the problem including all required steps and calculations.

Honors Section

The honors section of the course will have to complete additional assignments on some of the following topics:

- Gas adsorption
- Adsorption refrigeration
- Ideal adsorbed solution theory
- Joback method
- UNIFAC method
- Gamma-phi and phi-phi modeling
- Flash calculations for non-ideal solutions

The specific topics from this list will be identified by the instructor. The assignment will include both additional reading and problems. The problems will be assigned in the form of individual take-home exam. There will be up to three assignments during the semester.